

**WEST****End of Result Set**☐

Generate Collection

Print

L4: Entry 1 of 1

File: PGPB

Oct 3, 2002

DOCUMENT-IDENTIFIER: US 20020142108 A1

TITLE: Liquid crystal compounds, liquid crystal medium and liquid crystal display

Detail Description Table CWU (21):

25 Compound/Abbreviation Concentration/mass-% PTG-5-S 10.0 PTU-3-S 15.0 PTU-4O-S  
10.0 PVG-5-S 10.0 PGU-3-S 10.0 PPU-3-S 5.0 PPU-4-S 5.0 PPU-5-S 5.0 PGIP-3-N 15.0  
PPYP-4N 15.0 .SIGMA. 100.0

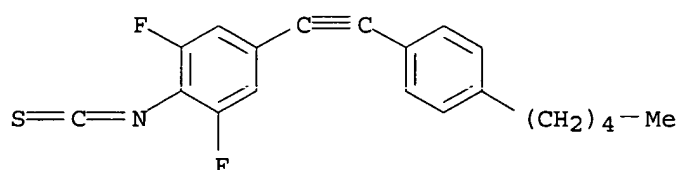
Detail Description Table CWU (23):

27 Compound/Abbreviation Concentration/mass-% PTG-5-S 10.0 PTU-3-S 13.0 PTU-4O-S  
10.0 PVG-5-S 11.0 PGU-3-S 10.0 PPU-3-S 5.0 PPU-4-S 5.0 PPU-5-S 5.0 PGIP-3-N 12.0  
PPYP-4N 13.0 PVG-V-S 6.0 .SIGMA. 100.0

RN 313472-50-3 REGISTRY  
 CN Benzene, 1,3-difluoro-2-isothiocyanato-5-[(4-pentylphenyl)ethynyl] - (9CI)  
 (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C20 H17 F2 N S  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

# Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C6	C6	6	C6	46.150.18	2



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
=====	=====	=====	=====
Bioconc. Factor (BCF)	1396095	pH 1	(1) ACD
Bioconc. Factor (BCF)	1396095	pH 4	(1) ACD
Bioconc. Factor (BCF)	1396095	pH 7	(1) ACD
Bioconc. Factor (BCF)	1396095	pH 8	(1) ACD
Bioconc. Factor (BCF)	1396095	pH 10	(1) ACD
Boiling Point (BP)	450.7+/-35.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	68.24+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	226.4+/-46.7 deg C		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	871159	pH 1	(1) ACD
Koc (KOC)	871159	pH 4	(1) ACD
Koc (KOC)	871159	pH 7	(1) ACD
Koc (KOC)	871159	pH 8	(1) ACD
Koc (KOC)	871159	pH 10	(1) ACD
logD (LOGD)	8.39	pH 1	(1) ACD
logD (LOGD)	8.39	pH 4	(1) ACD
logD (LOGD)	8.39	pH 7	(1) ACD
logD (LOGD)	8.39	pH 8	(1) ACD
logD (LOGD)	8.39	pH 10	(1) ACD
logP (LOGP)	8.388+/-0.512		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	341.42		(1) ACD
Vapor Pressure (VP)	6.87E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris

4 REFERENCES IN FILE CA (1957 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

## REFERENCE 1

AN 136:110201 CA  
 TI Liquid crystal compound, nematic liquid crystal mixture, and polymer dispersion liquid crystal display  
 IN Poetsch, Eike; Meyer, Volker; Krause, Joachim; Manabe, Atsutaka  
 PA Merck Patent G.M.B.H., Germany  
 SO Jpn. Kokai Tokkyo Koho, 40 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC ICM C09K019-42  
 ICS C09K019-12; C09K019-16; C09K019-30; G02F001-13; G02F001-1334  
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)  
 Section cross-reference(s): 75

## FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002012871	A2	20020115	JP 2001-137750	20010508
PRAI	EP 2000-109163		20000508		
AB	The invention relates to a nematic liq. crystal mixt. contg. a pos. anisotropic compd.(s) showing .DELTA.n of .gtoreq.0.30 (at 20.degree., 589.3 nm) represented by R1-A11-Z11-[A12-Z12]n-A13-NCS (R1 = C1-12-alky, Cl, OCF3, CN, NCS, F; Z11, Z12 = trans-CH:CH-, -CH:CF-, -CF:CH-, -CF:CF-, single bond; A11 = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-phenylene with F-substituent(s); A12, A13 = 1,4-phenylene, 1,4-phenylene with F-substituent(s); n = 0, 1) and a pos. anisotropic compd.(s) represented by R2-[A21]n-A22-A23-X2 (R2 = C1-12-alky, Cl, OCF3, CN, NCS, F; Z11, Z12 = trans-CH:CH-, -CH:CF-, -CF:CH-, -CF:CF-, single bond; A21 = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-phenylene with F-substituent(s); A22, A23 = 1,4-phenylene, 1,4-phenylene with F-substituent(s); X2 = CN, F, Cl; n = 0, 1). The liq. crystal mixt., showing wide-nematic-phase temp. ranges and low viscosity, is esp. suitable for (holog.) polymer dispersed liq. crystal displays.				
ST	nematic liq crystal mixt polymer dispersion display				
IT	Liquid crystal displays (nematic liq. crystal mixt. esp. suitable for holog. polymer dispersion liq. crystal display)				
IT	Liquid crystals (nematic; nematic liq. crystal mixt. esp. suitable for holog. polymer dispersion liq. crystal display)				
IT	38190-45-3	40817-08-1	52709-86-1	54211-46-0	63617-61-8
	99217-32-0	99602-91-2	104569-87-1	104569-88-2	116831-09-5
	132123-39-8	137019-94-4	137019-95-5	219939-28-3	219939-29-4
	281680-31-7	313472-50-3	316364-68-8	356797-91-6	356797-92-7
	356797-93-8	356797-97-2	356797-99-4	356798-03-3	356798-05-5
	356798-06-6	356798-12-4	356798-23-7	356798-25-9	356798-26-0
	356798-27-1	356798-31-7	356798-32-8	385435-70-1	388625-24-9
	388625-25-0	388625-26-1	388625-28-3	388625-29-4	388625-31-8
	388625-33-0	388625-42-1	388625-45-4		
	RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses) (nematic liq. crystal mixt. esp. suitable for holog. polymer dispersion liq. crystal display)				
IT	288-32-4, Imidazole, reactions 463-71-8, Thiophosgene 6160-65-2 67567-26-4, 4-Bromo-2,6-difluoroaniline 143651-26-7, Boronic acid, [4-(4-pentylcyclohexyl)phenyl]-, trans- 388623-07-2 388623-85-6				

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of nematic liq. crystal mixt. esp. suitable for holog. polymer  
 dispersion liq. crystal display)

IT	138074-14-3P	385435-64-3P	385435-68-7P	385435-69-8P	385435-73-4P
	388623-08-3P	388623-10-7P	388623-12-9P	388623-13-0P	388623-14-1P
	388623-15-2P	388623-17-4P	388623-18-5P	388623-19-6P	388623-20-9P
	388623-21-0P	388623-22-1P	388623-30-1P	388623-32-3P	388623-33-4P
	388623-34-5P	388623-35-6P	388623-36-7P	388623-37-8P	388623-38-9P
	388623-39-0P	388623-40-3P	388623-42-5P	388623-43-6P	388623-44-7P
	388623-45-8P	388623-46-9P	388623-47-0P	388623-49-2P	388623-50-5P
	388623-51-6P	388623-52-7P	388623-54-9P	388623-55-0P	388623-56-1P
	388623-57-2P	388623-58-3P	388623-59-4P	388623-60-7P	388623-62-9P
	388623-63-0P	388623-64-1P	388623-65-2P	388623-66-3P	388623-67-4P
	388623-68-5P	388623-69-6P	388623-70-9P	388623-71-0P	388623-72-1P
	388623-73-2P	388623-74-3P	388623-75-4P	388623-76-5P	388623-77-6P
	388623-78-7P	388623-79-8P	388623-80-1P	388623-82-3P	388623-83-4P
	388623-84-5P	388623-86-7P	388623-88-9P	388623-90-3P	388623-91-4P
	388623-93-6P	388623-94-7P	388623-95-8P	388623-96-9P	388623-97-0P
	388623-98-1P	388623-99-2P	388624-00-8P	388624-01-9P	388624-02-0P
	388624-03-1P	388624-04-2P	388624-05-3P	388624-07-5P	388624-08-6P
	388624-09-7P	388624-10-0P	388624-12-2P	388624-13-3P	388624-14-4P
	388624-15-5P	388624-16-6P	388624-17-7P	388624-18-8P	388624-19-9P
	388624-21-3P	388624-22-4P	388624-23-5P	388624-24-6P	388624-25-7P
	388624-26-8P	388624-27-9P	388624-28-0P	388624-29-1P	388624-31-5P
	388624-32-6P	388624-34-8P	388624-35-9P	388624-37-1P	388624-39-3P
	388624-40-6P	388624-42-8P	388624-43-9P	388624-44-0P	388624-46-2P
	388624-47-3P	388624-48-4P	388624-49-5P	388624-50-8P	388624-51-9P
	388624-52-0P	388624-53-1P	388624-54-2P	388624-55-3P	388624-56-4P
	388624-58-6P	388624-59-7P	388624-60-0P	388624-61-1P	388624-62-2P
	388624-63-3P	388624-64-4P	388624-65-5P	388624-66-6P	388624-67-7P
	388624-68-8P	388624-69-9P	388624-71-3P	388624-72-4P	388624-73-5P
	388624-74-6P	388624-75-7P	388624-76-8P	388624-77-9P	388624-78-0P
	388624-80-4P	388624-81-5P	388624-83-7P	388624-84-8P	388624-85-9P
	388624-86-0P	388624-92-8P	388624-93-9P	388624-94-0P	388624-95-1P
	388624-96-2P	388624-97-3P	388624-98-4P	388624-99-5P	388625-00-1P
	388625-01-2P	388625-02-3P	388625-03-4P	388625-04-5P	388625-05-6P
	388625-06-7P	388625-07-8P	388625-08-9P	388625-09-0P	388625-10-3P
	388625-11-4P	388625-12-5P	388625-13-6P	388625-14-7P	388625-15-8P
	388625-16-9P	388625-17-0P	388625-18-1P	388625-19-2P	388625-20-5P
	388625-21-6P	388625-22-7P	388625-23-8P		

RL: SPN (Synthetic preparation); TEM (Technical or engineered material  
 use); PREP (Preparation); USES (Uses)  
 (prepn. of nematic liq. crystal mixt. esp. suitable for holog. polymer  
 dispersion liq. crystal display)

#### REFERENCE 2

AN 136:77327 CA  
 TI Liquid-crystal medium, liquid-crystal display using it, and utilization of  
 it  
 IN Manabe, Atsutaka; Poetsch, Eike; Reiffenrath, Volker  
 PA Merck Patent G.M.B.H., Germany  
 SO Jpn. Kokai Tokkyo Koho, 27 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC ICM C09K019-02  
 ICS C09K019-12; C09K019-16; C09K019-18; C09K019-30; C09K019-34;  
 C09K019-42; G02F001-13; G02F001-1334  
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other  
 Reprographic Processes)

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----

PI JP 2002003844 A2 20020109 JP 2001-137708 20010508

PRAI EP 2000-109162 20000508

AB The medium contains (1) a strongly pos. dielec. liq.-crystal component A comprising .gtoreq.1 compds. having NCS groups at a terminal and having .DELTA.n >0.30 at 20.degree. and 589.3 nm and (2) a pos. dielec. liq.-crystal component B contg. compds. with broad nematic phase range. Also claimed are liq.-crystal displays and systems including the medium. The medium is esp. suitable for polymer dispersed liq.-crystal systems (PDLC) and holog. PDLC.

ST liq crystal display pos dielec component broad nematic phase

IT Liquid crystal displays

(liq.-crystal medium with strongly pos. dielec. and broad nematic phase range for display)

IT 40817-08-1D, mixt. contg. 52709-86-1D, mixt. contg. 58743-75-2D, mixt. contg. 58743-76-3D, mixt. contg. 99217-32-0D, mixt. contg. 116831-09-5D, mixt. contg. 138074-14-3D, mixt. contg. 313472-50-3D, mixt. contg. 316364-68-8D, mixt. contg. 356797-91-6D, mixt. contg. 356797-92-7D, mixt. contg. 356797-93-8D, mixt. contg. 356797-99-4D, mixt. contg. 356798-03-3D, mixt. contg. 356798-05-5D, mixt. contg. 356798-06-6D, mixt. contg. 356798-23-7D, mixt. contg. 356798-27-1D, mixt. contg. 385435-48-3 385435-64-3D, mixt. contg. 385435-68-7D, mixt. contg. 385435-69-8D, mixt. contg. 385435-70-1D, mixt. contg. 385435-71-2 385435-72-3 385435-73-4D, mixt. contg.

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(liq.-crystal medium with strongly pos. dielec. and broad nematic phase range for display)

#### REFERENCE 3

AN 135:203078 CA

TI Liquid crystal medium comprising strongly dielectric positive isothiocyanate compound for polymer dispersed liquid crystal display

IN Poetsch, Eike; Manabe, Atsutaka; Reiffenrath, Volker; Reuter, Markus; Krause, Joachim; Pauluth, Detlef

PA Merck Patent Gmbh, Germany

SO Eur. Pat. Appl., 54 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C09K019-02

ICS C09K019-16; C09K019-12; C09K019-42; C09K019-44; C09K019-54; C07C331-28

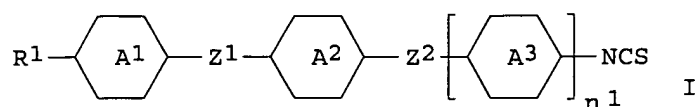
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1126006	A2	20010822	EP 2001-101157	20010123
	EP 1126006	A3	20030226		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	US 2002142108	A1	20021003	US 2001-773673	20010202
	JP 2001254080	<del>A2</del>	<del>200110918</del>	JP 2001-37730	20010214
PRAI	EP 2000-102952	20000214			
	EP 2000-109164	20000508			
	EP 2000-126408	20001205			
	EP 2000-EP00109164	20000508			
	EP 2000-EP00126408	20001205			

GI



AB The invention relates to liq. crystal media comprising a strongly dielec. pos. isothiocyanate compds. of formula I (R1=alkyl, C1-10-alkoxy, alkenyl, C1-7-alkenyloxy or-alkoxyalkyl, CN, NCS, halogen; Z1, Z2 = single bond, trans-CH=CH, Z2 = single bond if n1 = 0; n1 = 0,1; A1, A2, A3 = phenyls, at least one of phenyls is substituted by one or two fluorine atoms) , and another dielec. pos. compd., preferably comprising terminally polar substituted bi- or terphenyl compds., as further defined in the claims, as well as to liq. crystal displays comprising these media, in particular to polymer dispersed liq. crystal display (PDLC) and most particular to holog. PDLC displays.

ST liq crystal isothiocyanate compd medium prepn polymer dispersed display  
IT Liquid crystal displays  
Liquid crystals

(liq. crystal medium comprising strongly dielec. pos. isothiocyanate compds for polymer dispersed liq. crystal display)

IT 92-52-4, Biphenyl, reactions 367-24-8, 4-Bromo-2-fluoroaniline 461-96-1, 1-Bromo-3,5-difluoro-benzene 588-96-5, p-Ethoxyphenylbromide 5459-40-5, 4-Ethoxy-styrene 6160-65-2 6163-58-2, Tri-o-tolylphosphine 10101-89-0, Trisodiumphosphate dodecahydrate 13965-03-2 23055-77-8, 4-Bromo-4'-chloro-biphenyl 31989-57-8, Bis(triphenylphosphine) palladium 67567-26-4, 4-Bromo-2,6-difluoroaniline 105931-73-5, 1-Bromo-3-fluoro-4-iodo-benzene

RL: RCT (Reactant); RACT (Reactant or reagent)  
(in prepn. of isothiocyanate liq. crystal compds)

IT 71274-84-5P, 4-Trifluoromethoxy-biphenyl  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in prepn. of isothiocyanate liq. crystal compds)

IT 160347-36-4P 356797-91-6P 356797-92-7P 356797-93-8P 356797-94-9P  
356797-95-0P 356797-96-1P 356797-97-2P 356797-98-3P 356797-99-4P  
356798-00-0P 356798-01-1P 356798-02-2P 356798-03-3P 356798-04-4P  
356798-05-5P 356798-06-6P 356798-07-7P 356798-08-8P 356798-09-9P  
356798-10-2P 356798-11-3P 356798-12-4P 356798-13-5P 356798-14-6P  
356798-15-7P 356798-16-8P 356798-17-9P 356798-18-0P 356798-19-1P  
356798-20-4P 356798-21-5P 356798-22-6P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(liq. crystal medium comprising strongly dielec. pos. isothiocyanate compds for polymer dispersed liq. crystal display)

IT 63617-61-8 116831-09-5 127523-43-7 219939-28-3 219939-29-4  
313472-50-3 356798-23-7 356798-24-8 356798-25-9 356798-26-0  
356798-27-1 356798-28-2 356798-29-3 356798-30-6 356798-31-7  
356798-32-8

RL: TEM (Technical or engineered material use); USES (Uses)

(liq. crystal medium comprising strongly dielec. pos. isothiocyanate compds for polymer dispersed liq. crystal display)

#### REFERENCE 4

AN 134:63754 CA  
TI Materials for liquid crystal displays with reduced power consumption  
AU Kirsch, Peer; Bremer, Matthias; Kirsch, Annette; Manabe, Atsutaka; Poetsch, Eike; Reiffenrath, Volker; Tarumi, Kazuaki  
CS Liquid Crystals Division, Merck KGaA, Darmstadt, 64271, Germany  
SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (2000), 346, 193-199  
CODEN: MCLCE9; ISSN: 1058-725X

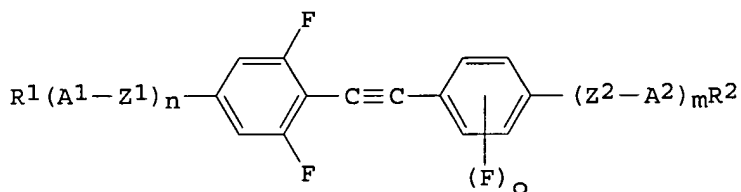
PB Gordon & Breach Science Publishers  
 DT Journal  
 LA English  
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)  
 Section cross-reference(s): 75  
 AB A significant redn. of the power consumption of a liq. crystal display can be achieved either by application of a lower driving voltage or - even more effectively - by use of a holog. structured reflective scattering type of display without color filters. The first option requires strongly polar materials with extremely high reliability, the second one new types of liq. crystals with a birefringence as high as possible in order to optimize the scattering effect. A mol. modeling based method for the prediction of reliability parameters is presented.  
 ST liq crystal display active matrix high birefringence reliability material; mol model stable materials liq crystal display active matrix  
 IT Liquid crystal displays  
 (active matrix; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption)  
 IT Ion-molecule reaction  
 (enthalpy, calcd. semiempirical; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)  
 IT Liquid crystals  
 (fluorinated; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)  
 IT Reaction enthalpy  
 (ion-mol. reaction, calcd. semiempirical; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)  
 IT Impurities  
 (ionic; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to)  
 IT Birefringence  
 Dielectric anisotropy  
 (materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption)  
 IT Molecular modeling  
 (materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption supported by)  
 IT Molecular structure-property relationship  
 (stability; materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to materials stability)  
 IT 126391-77-3 133261-31-1 221526-80-3 255728-73-5 255728-82-6  
 308117-08-0 313472-49-0 313472-50-3  
 RL: PRP (Properties)  
 (materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption)  
 IT 17341-25-2, processes  
 RL: PEP (Physical, engineering or chemical process); PROC (Process)  
 (materials with high birefringence or improved voltage holding ratio for active matrix liq. crystal displays with reduced power consumption in relation to ionic impurities)  
 RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 (1) Bremer, M; Adv Mater 1993, V5, P842 CAPLUS  
 (2) Bremer, M; Jpn J Appl Phys 1998, V37, PL88 CAPLUS  
 (3) Kirsch, P; Angew Chem 1999, V111, P2174  
 (4) Kirsch, P; Angew Chem Int Ed Engl 1999, V38, P1989 CAPLUS  
 (5) Klasen, M; Jpn J Appl Phys 1998, V37, PL945 CAPLUS

(6) Sasaki, A; Japan Display '86 1986, P62



AN 1993:59406 CAPLUS  
 DN 118:59406  
 TI 2,6 difluorotolane  
 IN Reiffenrath, Volker; Plach, Herbert  
 PA Merck Patent G.m.b.H., Germany  
 SO Ger. Offen., 19 pp.  
 CODEN: GWXXBX  
 DT Patent  
 LA German  
 IC ICM C07C043-225  
 ICS C07C025-24; C09K019-06; G09F009-35; G02F001-13; C07D319-06;  
 C07D213-24; C07D239-24  
 ICA C09K019-18; C09K019-30; C09K019-34; C09K019-20; C09K019-58; C07D521-00;  
 C07D401-10; C07D401-12; C07D405-10; C07D405-12  
 CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4105742	A1	19920827	DE 1991-4105742	19910223
	DE 4105742	C2	20010809		
PRAI	DE 1991-4105742		19910223		
OS	CASREACT 118:59406; MARPAT 118:59406				
GI					



AB A process was developed for the prepn. of 2,6-difluorotolane of formula I [R1, R2 = alkyl or alkenyl, A1, A2 = 1,4-cyclohexylene, -phenylene, 2- or 3-fluoro-1,4-phenylene, Z1, Z2 = CH2CH2, -CH2O-, (CH2)4, m, n, o = 1-2] as a component of liq. crystal medium having electrooptical properties. E.g., the treatment of 3,5-difluoropentylbenzene (0.129 mol) with 114 mL THF and BuLi followed by 4-ethoxyacetophenone (0.129 mol) gave a product mixt. which was treated with p-toluenesulfonic acid (4 g) in toluene. Subsequent reaction of product mixt. with .09 mL bromine in EtOAc and with 12.6 mL Et3N and then reaction with LDA in THF gave final product 4-pentyl-2,6-difluoro-4'-ethoxytolane.

ST fluorotolane electrooptical property; acetylene difluoro diphenyl;  
 palladium catalyst coupling fluorophenylacetylene iodobenzene

IT Coupling reaction  
 (of difluorophenylacetylene with trifluoromethoxyiodobenzene and  
 analogs, difluorotolanes from)

IT Coupling reaction catalysts  
 (palladium compds., for the coupling of difluorophenylacetylene with  
 trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT 144890-97-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (3)

IT 14221-01-3  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst, for the coupling of difluoroiodobenzene derivs. with  
 fluorophenylacetylene)

IT 13965-03-2  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst, for the coupling of difluorophenylacetylene deriv. with  
 trifluoromethoxyiodobenzene)

IT 628-17-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction of, with difluorobromobenzene)

IT 461-96-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction of, with iodopentane)

IT 103962-05-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction of, with difluorophenylacetylene deriv.)

IT 766-98-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction of, with ethoxydifluoriodobenzene)

IT 144911-50-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction of, with trifluoromethoxyiodobenzene)

IT 144891-25-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(iodination of)

IT 144891-24-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and coupling of, with fluorophenylacetylene)

IT 40817-08-1P 41122-70-7P 52709-83-8P 58743-75-2P 58743-76-3P  
61203-99-4P 61204-01-1P 79832-84-1P 80944-44-1P 80955-71-1P  
81936-32-5P 85600-56-2P 134143-76-3P 144890-96-0P 144890-98-2P  
144890-99-3P 144891-00-9P 144891-01-0P 144891-02-1P 144891-03-2P  
144891-04-3P 144891-05-4P 144891-06-5P 144891-07-6P 144891-08-7P  
144891-09-8P 144891-10-1P 144891-11-2P 144891-12-3P 144891-13-4P  
144891-14-5P 144891-15-6P 144891-16-7P 144891-17-8P 144891-18-9P  
144891-19-0P 144891-20-3P 144891-21-4P 144891-22-5P 144891-23-6P  
144891-26-9P 144891-27-0P 144891-28-1P 144891-29-2P 144891-30-5P  
144891-31-6P 144891-32-7P **144891-33-8P 144891-34-9P**  
**144891-35-0P 144891-36-1P 144891-37-2P**  
**144891-38-3P 144891-39-4P 144891-40-7P 144891-41-8P**  
144891-42-9P 144891-43-0P 144891-44-1P 144891-45-2P 144891-46-3P  
144891-47-4P 144891-48-5P 144891-49-6P 144891-50-9P 144891-51-0P  
144891-52-1P 144891-53-2P 144891-54-3P 144891-55-4P 144891-56-5P  
144891-57-6P 144891-58-7P 144891-59-8P 144891-60-1P 144891-61-2P  
144891-62-3P 144891-63-4P 144891-64-5P 144891-65-6P 144891-66-7P  
144891-67-8P 144891-68-9P 144891-69-0P 144891-70-3P 144891-71-4P  
144891-72-5P 144891-73-6P 144891-74-7P 144891-75-8P 144891-76-9P  
144891-77-0P 144891-78-1P 144891-79-2P 144891-80-5P 144891-81-6P  
144891-82-7P 144891-83-8P 144891-84-9P 144891-85-0P 144891-86-1P  
144891-87-2P 144891-88-3P 144891-89-4P 144891-90-7P 144891-91-8P  
144891-92-9P 144891-93-0P 144891-94-1P 144891-95-2P 144891-96-3P  
144891-97-4P 144891-98-5P 144891-99-6P 144892-00-2P 144892-01-3P  
144892-02-4P 144892-03-5P 144892-04-6P 144892-05-7P 144892-06-8P  
144892-07-9P 144892-08-0P 144892-09-1P 144892-10-4P 144892-11-5P  
144892-12-6P 144892-13-7P 144892-14-8P 144892-15-9P 144892-16-0P  
144892-17-1P 144892-18-2P 144892-19-3P 144892-20-6P 144892-21-7P  
144892-22-8P 144892-23-9P 144892-24-0P 144892-25-1P 144892-26-2P  
144892-27-3P 144892-28-4P 144892-29-5P 144892-30-8P 144892-31-9P  
144892-32-0P 144892-33-1P 144892-34-2P 144892-35-3P 144892-36-4P  
144892-37-5P 144892-38-6P 144892-39-7P 144892-40-0P 144892-41-1P  
144892-42-2P 144892-43-3P 144892-44-4P 144892-45-5P 144892-46-6P  
144892-47-7P 144892-48-8P 144892-49-9P 144892-50-2P 144892-51-3P  
144892-52-4P 144892-53-5P 144892-54-6P 144892-55-7P 144892-56-8P  
144892-57-9P 144892-58-0P 144892-59-1P 144892-60-4P 144892-61-5P  
144892-62-6P 144892-63-7P 144911-05-7P 144911-06-8P 144911-07-9P  
144911-08-0P 144911-09-1P 144911-10-4P 144911-11-5P 144911-12-6P  
144911-13-7P 144911-14-8P 144911-15-9P 144911-16-0P 144911-17-1P  
144911-18-2P 144911-19-3P 144911-20-6P 144911-21-7P 144911-22-8P  
144911-23-9P 144911-24-0P 144911-25-1P 144911-26-2P 144911-27-3P  
144911-28-4P 144911-29-5P 144911-30-8P 144911-31-9P 144911-32-0P

144911-33-1P 144911-34-2P 144911-35-3P 144911-36-4P 144911-37-5P  
 144911-38-6P 144911-39-7P 144911-40-0P 144911-41-1P 144911-42-2P  
 144911-43-3P 144911-44-4P 144911-45-5P 144911-46-6P 144911-47-7P  
 144911-48-8P 144911-49-9P 144911-51-3P 144911-52-4P 144911-53-5P  
 144911-54-6P 144911-55-7P 144911-56-8P **144911-57-9P**  
**144911-58-0P 144911-59-1P 144911-60-4P**  
**144911-61-5P 144911-62-6P 144911-63-7P**  
 144911-64-8P 144911-65-9P 144911-66-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

IT 144911-67-1P 144911-68-2P 144911-69-3P 144911-70-6P 144911-71-7P  
 144911-72-8P 144911-73-9P 144911-74-0P 144922-37-2P 144922-38-3P  
 144922-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

IT 1676-63-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with difluoro(pentyl)benzene)

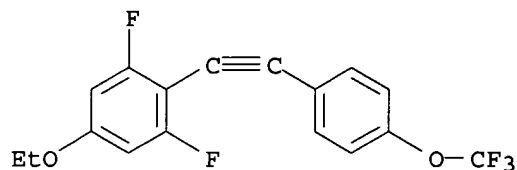
IT 121219-25-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with ethoxyacetophenone)

IT **144891-33-8P 144891-34-9P 144891-35-0P**  
**144891-36-1P 144891-37-2P 144891-38-3P**  
**144891-39-4P 144911-57-9P 144911-58-0P**  
**144911-59-1P 144911-60-4P 144911-61-5P**  
**144911-62-6P 144911-63-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

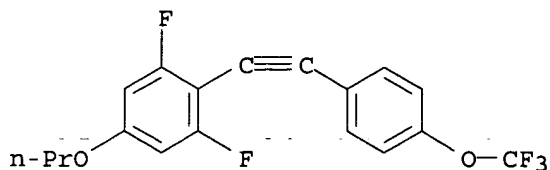
RN 144891-33-8 CAPLUS

CN Benzene, 5-ethoxy-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



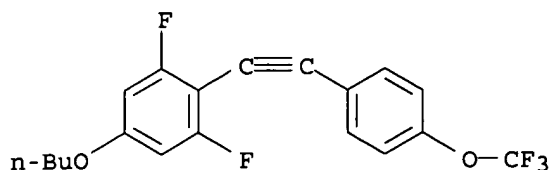
RN 144891-34-9 CAPLUS

CN Benzene, 1,3-difluoro-5-propoxy-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)

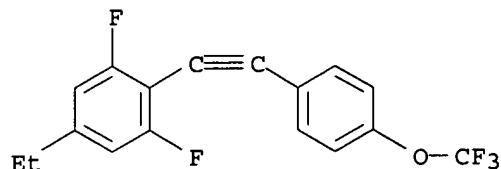


RN 144891-35-0 CAPLUS

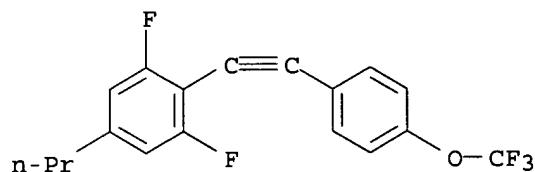
CN Benzene, 5-butoxy-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



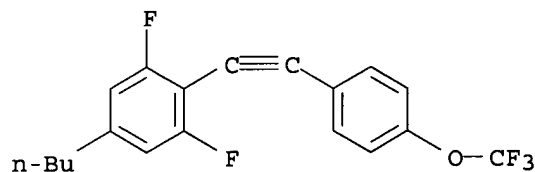
RN 144891-36-1 CAPLUS  
 CN Benzene, 5-ethyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



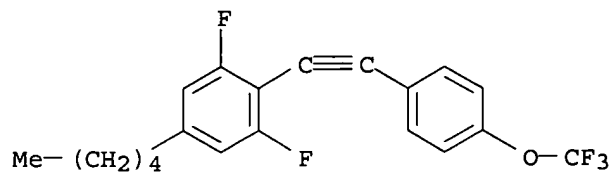
RN 144891-37-2 CAPLUS  
 CN Benzene, 1,3-difluoro-5-propyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



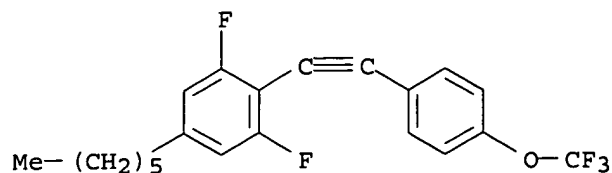
RN 144891-38-3 CAPLUS  
 CN Benzene, 5-butyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



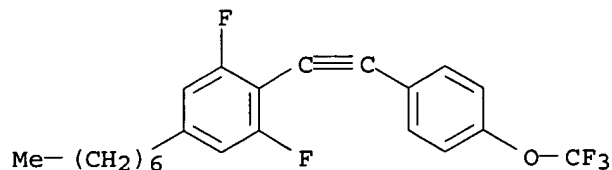
RN 144891-39-4 CAPLUS  
 CN Benzene, 1,3-difluoro-5-pentyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



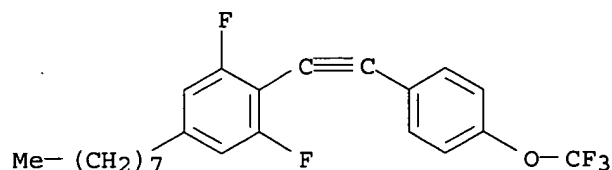
RN 144911-57-9 CAPLUS  
 CN Benzene, 1,3-difluoro-5-hexyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



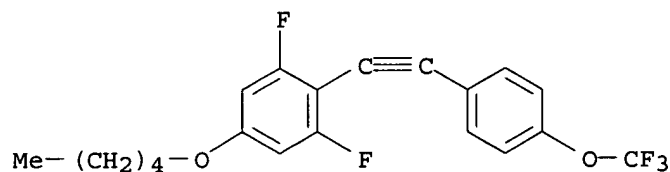
RN 144911-58-0 CAPLUS  
 CN Benzene, 1,3-difluoro-5-heptyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



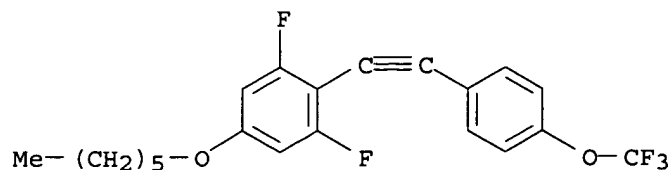
RN 144911-59-1 CAPLUS  
 CN Benzene, 1,3-difluoro-5-octyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



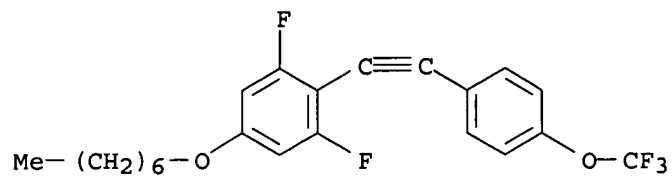
RN 144911-60-4 CAPLUS  
 CN Benzene, 1,3-difluoro-5-(pentyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 ]- (9CI) (CA INDEX NAME)



RN 144911-61-5 CAPLUS  
 CN Benzene, 1,3-difluoro-5-(hexyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)

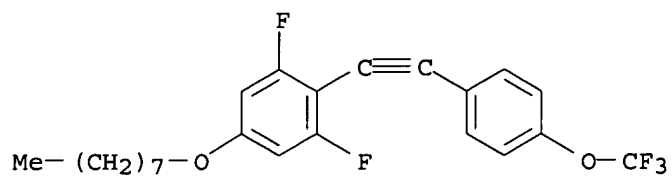


RN 144911-62-6 CAPLUS  
 CN Benzene, 1,3-difluoro-5-(heptyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 ]- (9CI) (CA INDEX NAME)

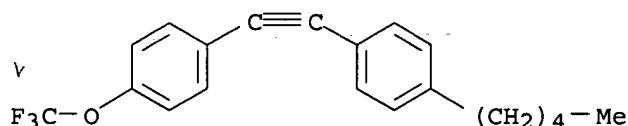


RN 144911-63-7 CAPLUS

CN Benzene, 1,3-difluoro-5-(octyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
(9CI) (CA INDEX NAME)



AN 1990:641336 CAPLUS  
 DN 113:241336  
 TI Synthesis and properties of liquid crystalline materials with high optical anisotropy  
 AU Reiffenrath, V.; Finkenzeller, U.; Poetsch, E.; Rieger, B.; Coates, D.  
 CS Ind. Chem. Div., E. Merck, Darmstadt, D-6100, Germany  
 SO Proceedings of SPIE-The International Society for Optical Engineering (1990), 1257(Liq. Cryst. Disp. Appl.), 84-94  
 CODEN: PSISDG; ISSN: 0277-786X  
 DT Journal  
 LA English  
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)  
 Section cross-reference(s): 21, 75  
 AB The introduction of F and F-contg. substituents in the terminal position of high .DELTA.n (refractive index difference) materials leads to liq. crystals with high pos. dielec. anisotropy and low viscosity. These liq. crystals exhibit high resistivity and excellent UV-stability. In contrast to the cyano-substituent these moieties do not enhance the optical anisotropy; therefore the use of basic structures having high optical anisotropy such as tolans and terphenyls is necessary. In the case of terphenyls the introduction of an ethylenic bridge in addn. to lateral fluorination leads to mols. having a wide nematic phase range.  
 ST synthesis liq crystal optical anisotropy; electrooptical device liq crystal dielec anisotropy  
 IT Liquid crystals  
 (prepn. of fluorine-contg., with high optical anisotropy and UV stability and low viscosity)  
 IT Optical imaging devices  
 (electro-, liq.-crystal, prepn. of fluorine-contg. liq. crystal materials having high optical anisotropy and UV stability and low viscosity for)  
 IT 95759-62-9P 116903-47-0P 121218-93-7P 130746-59-7P  
 130746-60-0P 130746-61-1P 130746-62-2P  
 130746-63-3P 130746-64-4P 130746-65-5P 130746-66-6P  
 130746-67-7P 130746-68-8P 130746-69-9P 130746-70-2P 130746-71-3P  
 130746-72-4P 130746-73-5P 130746-74-6P 130746-75-7P 130746-76-8P  
 130746-77-9P 130746-78-0P 130746-79-1P 130746-80-4P 130746-81-5P  
 RL: PREP (Preparation)  
 (prepn. and dielec. anisotropy and UV stability and viscosity of, for display devices)  
 IT 130746-60-0P 130746-62-2P 130746-63-3P  
 RL: PREP (Preparation)  
 (prepn. and dielec. anisotropy and UV stability and viscosity of, for display devices)  
 RN 130746-60-0 CAPLUS  
 CN Benzene, 1-[(4-pentylphenyl)ethynyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



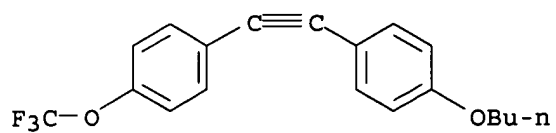
RN 130746-62-2 CAPLUS  
 CN Benzene, 1-[(4-butoxyphenyl)ethynyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

X

not

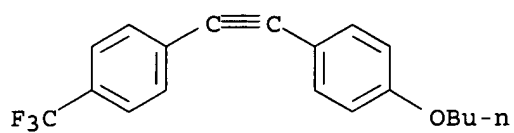
F

at my

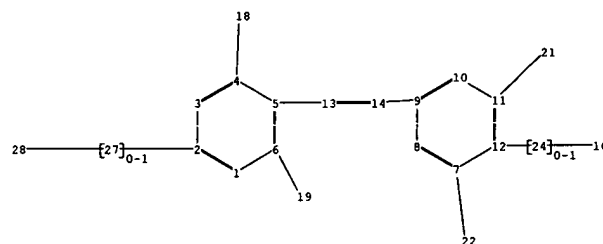
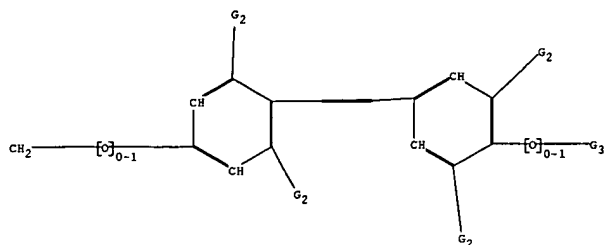


RN 130746-63-3 CAPLUS

CN Benzene, 1-[(4-butoxyphenyl)ethynyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)







chain nodes :

13 14 16 18 19 21 22 24 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

2-27 4-18 5-13 6-19 7-22 9-14 11-21 12-24 13-14 16-24 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

2-27 4-18 6-19 7-22 11-21 12-24 16-24

exact bonds :

5-13 9-14 13-14 27-28

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

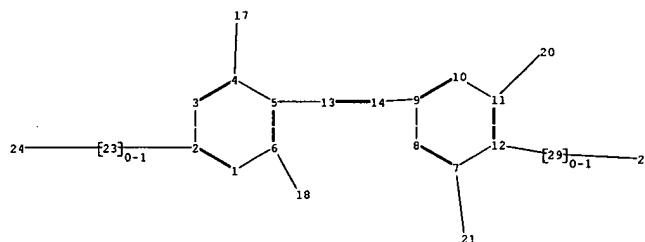
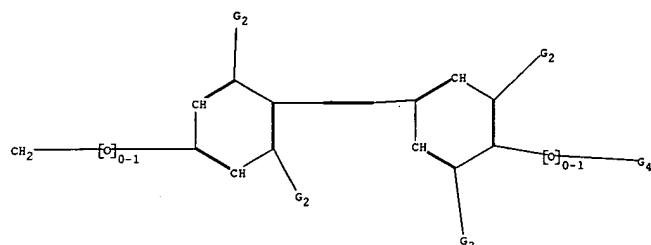
G1:C,O

G2:H,F

G3:CF3,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:CLASS 14:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 24:CLASS  
27:CLASS 28:CLASS



chain nodes :

13 14 17 18 20 21 23 24 28 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

2-23 4-17 5-13 6-18 7-21 9-14 11-20 12-29 13-14 23-24 28-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

2-23 4-17 6-18 7-21 11-20 12-29 28-29

exact bonds :

5-13 9-14 13-14 23-24

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:C,O

G2:H,F

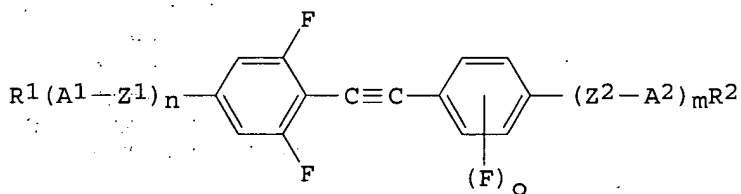
G3:CN,CF<sub>3</sub>,NG4:CF<sub>3</sub>,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:CLASS 14:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS 23:CLASS 24:CLASS  
 28:CLASS 29:CLASS

AN 1993:59406 CAPLUS  
 DN 118:59406  
 TI 2,6 difluorotolane  
 IN Reiffenrath, Volker; Plach, Herbert  
 PA Merck Patent G.m.b.H., Germany  
 SO Ger. Offen., 19 pp.  
 CODEN: GWXXBX  
 DT Patent  
 LA German  
 IC ICM C07C043-225  
 ICS C07C025-24; C09K019-06; G09F009-35; G02F001-13; C07D319-06;  
 C07D213-24; C07D239-24  
 ICA C09K019-18; C09K019-30; C09K019-34; C09K019-20; C09K019-58; C07D521-00;  
 C07D401-10; C07D401-12; C07D405-10; C07D405-12  
 CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4105742	A1	19920827	DE 1991-4105742	19910223
	DE 4105742	C2	20010809		
PRAI	DE 1991-4105742		19910223		
OS	CASREACT 118:59406; MARPAT 118:59406				
GI					



AB A process was developed for the prepn. of 2,6-difluorotolane of formula I [R1, R2 = alkyl or alkenyl, A1, A2 = 1,4-cyclohexylene, -phenylene, 2- or 3-fluoro-1,4-phenylene, Z1, Z2 = CH2CH2, -CH2O-, (CH2)4, m, n, o = 1-2] as a component of liq. crystal medium having electrooptical properties. E.g., the treatment of 3,5-difluoropentylbenzene (0.129 mol) with 114 mL THF and BuLi followed by 4-ethoxyacetophenone (0.129 mol) gave a product mixt. which was treated with p-toluenesulfonic acid (4 g) in toluene. Subsequent reaction of product mixt. with .09 mL bromine in EtOAc and with 12.6 mL Et3N and then reaction with LDA in THF gave final product 4-pentyl-2,6-difluoro-4'-ethoxytolane.

ST fluorotolane electrooptical property; acetylene difluoro diphenyl; palladium catalyst coupling fluorophenylacetylene iodobenzene

IT Coupling reaction  
 (of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT Coupling reaction catalysts  
 (palladium compds., for the coupling of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT 144890-97-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (3)

IT 14221-01-3  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst, for the coupling of difluoroidobenzene derivs. with fluorophenylacetylene)

IT 13965-03-2  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst, for the coupling of difluorophenylacetylene deriv. with trifluoromethoxyiodobenzene)

IT 628-17-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction of, with difluorobromobenzene)

IT 461-96-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction of, with iodopentane)

IT 103962-05-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction of, with difluorophenylacetylene deriv.)

IT 766-98-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction of, with ethoxydifluoriodobenzene)

IT 144911-50-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling reaction of, with trifluoromethoxyiodobenzene)

IT 144891-25-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(iodination of)

IT 144891-24-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and coupling of, with fluorophenylacetylene)

IT 40817-08-1P 41122-70-7P 52709-83-8P 58743-75-2P 58743-76-3P  
61203-99-4P 61204-01-1P 79832-84-1P 80944-44-1P 80955-71-1P  
81936-32-5P 85600-56-2P 134143-76-3P 144890-96-0P 144890-98-2P  
144890-99-3P 144891-00-9P 144891-01-0P 144891-02-1P 144891-03-2P  
144891-04-3P 144891-05-4P 144891-06-5P 144891-07-6P 144891-08-7P  
144891-09-8P 144891-10-1P 144891-11-2P 144891-12-3P 144891-13-4P  
144891-14-5P 144891-15-6P 144891-16-7P 144891-17-8P 144891-18-9P  
144891-19-0P 144891-20-3P 144891-21-4P 144891-22-5P 144891-23-6P  
144891-26-9P 144891-27-0P 144891-28-1P 144891-29-2P 144891-30-5P  
144891-31-6P 144891-32-7P 144891-33-8P 144891-34-9P  
144891-35-0P 144891-36-1P 144891-37-2P  
144891-38-3P 144891-39-4P 144891-40-7P 144891-41-8P  
144891-42-9P 144891-43-0P 144891-44-1P 144891-45-2P 144891-46-3P  
144891-47-4P 144891-48-5P 144891-49-6P 144891-50-9P 144891-51-0P  
144891-52-1P 144891-53-2P 144891-54-3P 144891-55-4P 144891-56-5P  
144891-57-6P 144891-58-7P 144891-59-8P 144891-60-1P 144891-61-2P  
144891-62-3P 144891-63-4P 144891-64-5P 144891-65-6P 144891-66-7P  
144891-67-8P 144891-68-9P 144891-69-0P 144891-70-3P 144891-71-4P  
144891-72-5P 144891-73-6P 144891-74-7P 144891-75-8P 144891-76-9P  
144891-77-0P 144891-78-1P 144891-79-2P 144891-80-5P 144891-81-6P  
144891-82-7P 144891-83-8P 144891-84-9P 144891-85-0P 144891-86-1P  
144891-87-2P 144891-88-3P 144891-89-4P 144891-90-7P 144891-91-8P  
144891-92-9P 144891-93-0P 144891-94-1P 144891-95-2P 144891-96-3P  
144891-97-4P 144891-98-5P 144891-99-6P 144892-00-2P 144892-01-3P  
144892-02-4P 144892-03-5P 144892-04-6P 144892-05-7P 144892-06-8P  
144892-07-9P 144892-08-0P 144892-09-1P 144892-10-4P 144892-11-5P  
144892-12-6P 144892-13-7P 144892-14-8P 144892-15-9P 144892-16-0P  
144892-17-1P 144892-18-2P 144892-19-3P 144892-20-6P 144892-21-7P  
144892-22-8P 144892-23-9P 144892-24-0P 144892-25-1P 144892-26-2P  
144892-27-3P 144892-28-4P 144892-29-5P 144892-30-8P 144892-31-9P  
144892-32-0P 144892-33-1P 144892-34-2P 144892-35-3P 144892-36-4P  
144892-37-5P 144892-38-6P 144892-39-7P 144892-40-0P 144892-41-1P  
144892-42-2P 144892-43-3P 144892-44-4P 144892-45-5P 144892-46-6P  
144892-47-7P 144892-48-8P 144892-49-9P 144892-50-2P 144892-51-3P  
144892-52-4P 144892-53-5P 144892-54-6P 144892-55-7P 144892-56-8P  
144892-57-9P 144892-58-0P 144892-59-1P 144892-60-4P 144892-61-5P  
144892-62-6P 144892-63-7P 144911-05-7P 144911-06-8P 144911-07-9P  
144911-08-0P 144911-09-1P 144911-10-4P 144911-11-5P 144911-12-6P  
144911-13-7P 144911-14-8P 144911-15-9P 144911-16-0P 144911-17-1P  
144911-18-2P 144911-19-3P 144911-20-6P 144911-21-7P 144911-22-8P  
144911-23-9P 144911-24-0P 144911-25-1P 144911-26-2P 144911-27-3P  
144911-28-4P 144911-29-5P 144911-30-8P 144911-31-9P 144911-32-0P

144911-33-1P 144911-34-2P 144911-35-3P 144911-36-4P 144911-37-5P  
 144911-38-6P 144911-39-7P 144911-40-0P 144911-41-1P 144911-42-2P  
 144911-43-3P 144911-44-4P 144911-45-5P 144911-46-6P 144911-47-7P  
 144911-48-8P 144911-49-9P 144911-51-3P 144911-52-4P 144911-53-5P  
 144911-54-6P 144911-55-7P 144911-56-8P 144911-57-9P  
 144911-58-0P 144911-59-1P 144911-60-4P  
 144911-61-5P 144911-62-6P 144911-63-7P  
 144911-64-8P 144911-65-9P 144911-66-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

IT 144911-67-1P 144911-68-2P 144911-69-3P 144911-70-6P 144911-71-7P  
 144911-72-8P 144911-73-9P 144911-74-0P 144922-37-2P 144922-38-3P  
 144922-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

IT 1676-63-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with difluoro(pentyl)benzene)

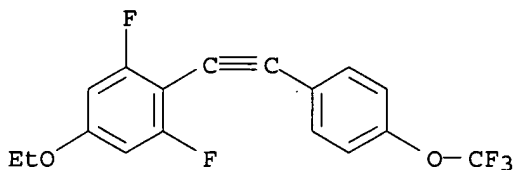
IT 121219-25-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with ethoxyacetophenone)

IT 144891-33-8P 144891-34-9P 144891-35-0P  
 144891-36-1P 144891-37-2P 144891-38-3P  
 144891-39-4P 144911-57-9P 144911-58-0P  
 144911-59-1P 144911-60-4P 144911-61-5P  
 144911-62-6P 144911-63-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

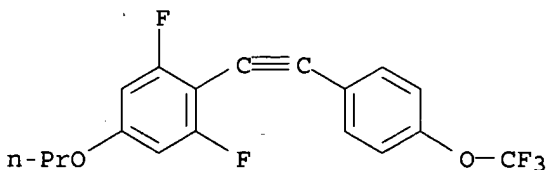
RN 144891-33-8 CAPLUS

CN Benzene, 5-ethoxy-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



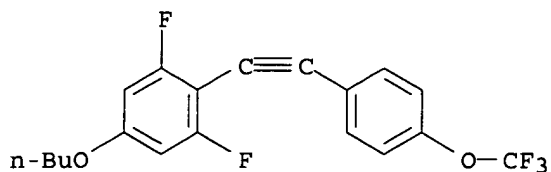
RN 144891-34-9 CAPLUS

CN Benzene, 1,3-difluoro-5-propoxy-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)

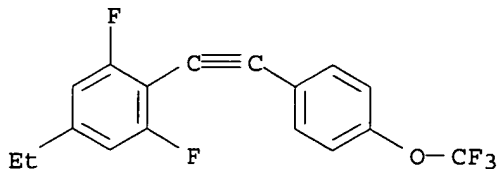


RN 144891-35-0 CAPLUS

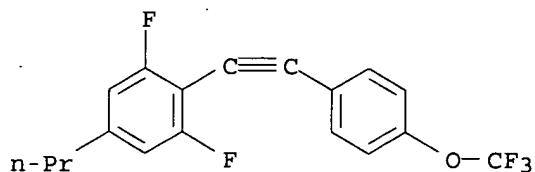
CN Benzene, 5-butoxy-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



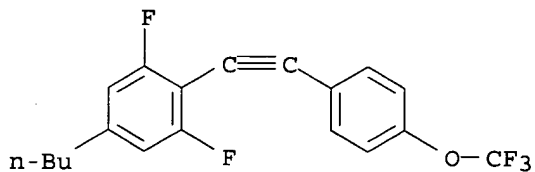
RN 144891-36-1 CAPLUS  
 CN Benzene, 5-ethyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



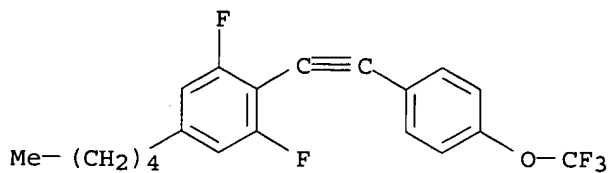
RN 144891-37-2 CAPLUS  
 CN Benzene, 1,3-difluoro-5-propyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



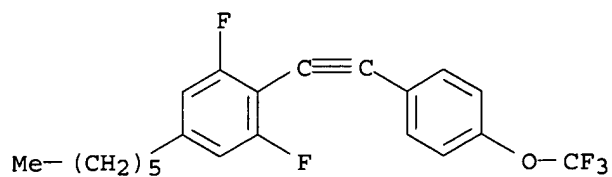
RN 144891-38-3 CAPLUS  
 CN Benzene, 5-butyl-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



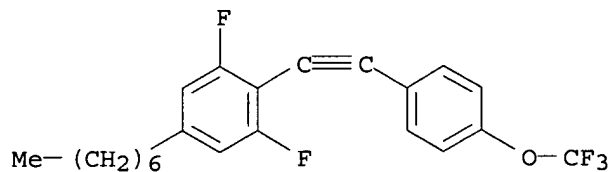
RN 144891-39-4 CAPLUS  
 CN Benzene, 1,3-difluoro-5-pentyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



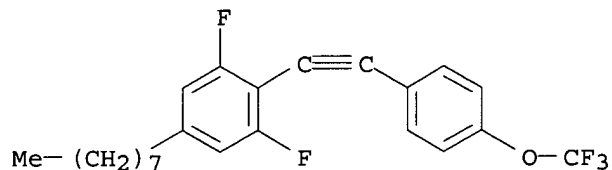
RN 144911-57-9 CAPLUS  
 CN Benzene, 1,3-difluoro-5-hexyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl] -  
 (9CI) (CA INDEX NAME)



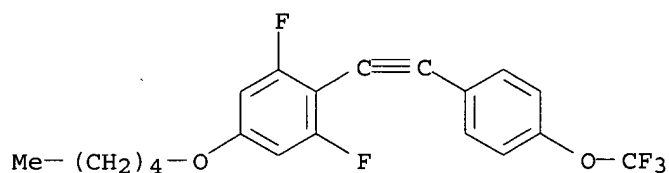
RN 144911-58-0 CAPLUS  
 CN Benzene, 1,3-difluoro-5-heptyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



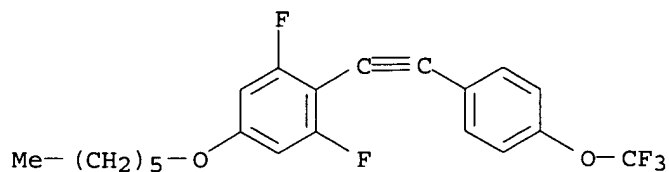
RN 144911-59-1 CAPLUS  
 CN Benzene, 1,3-difluoro-5-octyl-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



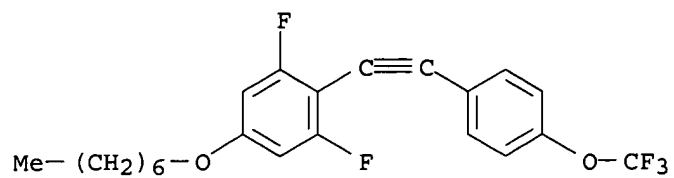
RN 144911-60-4 CAPLUS  
 CN Benzene, 1,3-difluoro-5-(pentyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



RN 144911-61-5 CAPLUS  
 CN Benzene, 1,3-difluoro-5-(hexyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



RN 144911-62-6 CAPLUS  
 CN Benzene, 1,3-difluoro-5-(heptyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
 (9CI) (CA INDEX NAME)



RN 144911-63-7 CAPLUS

CN Benzene, 1,3-difluoro-5-(octyloxy)-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-  
(9CI) (CA INDEX NAME)

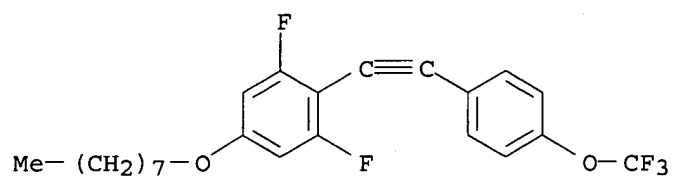
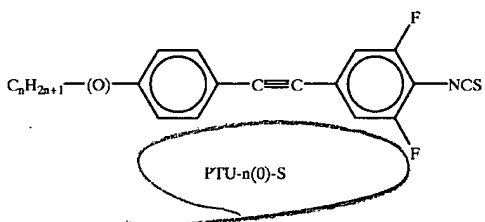
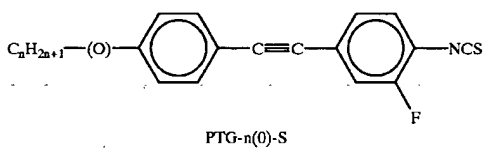
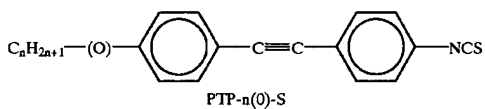
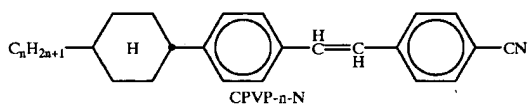
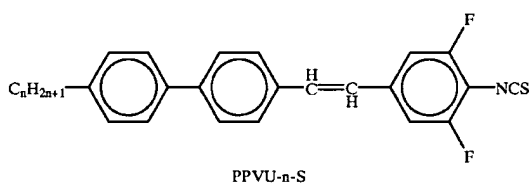
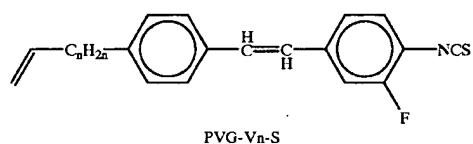
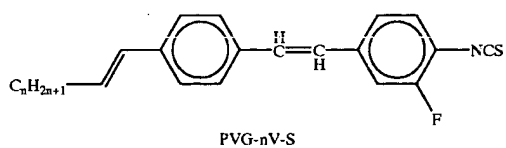
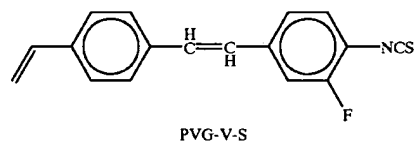
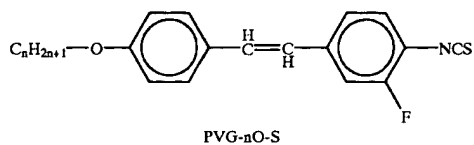




TABLE B-continued



## Use-example 7

[0216] A liquid crystal mixture is realized consisting of:

Compound/Abbreviation	Concentration/mass-%
PTG-5-S	10.0
PTU-3-S	15.0
PTU-4O-S	10.0
PVG-5-S	10.0
PGU-3-S	10.0
PPU-3-S	5.0
PPU-4-S	5.0
PPU-5-S	5.0
PGIP-3-N	15.0
PPYP-4N	15.0
$\Sigma$	100.0

[0217] This mixture has the following properties:

Clearing point (T(N,I))° C.:	126.5
Smectic to nematic transition point (T(S,N))° C.:	<-10
$n_e$ (20° C., 589.3 nm):	1.9475
$\Delta n$ (20° C., 589.3 nm):	0.4016

## Use-example 8

[0218] A liquid crystal mixture is realized consisting of:

Compound/Abbreviation	Concentration/mass-%
PTG-5-S	10.0
PTU-3-S	13.0
PTU-4O-S	10.0
PVG-5-S	11.0
PGU-3-S	10.0
PPU-3-S	5.0
PPU-4-S	5.0
PPU-5-S	5.0
PGIP-3-N	12.0
PPYP-4N	13.0
PVG-V-S	6.0
$\Sigma$	100.0

[0219] This mixture has the following properties:

Clearing point (T(N,I))° C.:	125.0
Smectic to nematic transition point (T(S,N))° C.:	<-10
$n_e$ (20° C., 589.3 nm):	1.9623
$\Delta n$ (20° C., 589.3 nm):	0.4153

## Use-example 9

[0220] A liquid crystal mixture is realized consisting of:

Compound/Abbreviation	Concentration/mass-%
PG-3-AN	8.0
PU-3-AN	7.0
PU-5-AN	7.0
PPVU-2-S	6.0
PPVU-3-S	6.0
PGP-3-N	6.0
PGIP-3-N	6.0
PPYP-4N	8.0
PTP-3-S	4.0
PTG-3-S	5.0
PVG-5-S	10.0
PTPG-2-N	4.0
PPU-CL-S	4.0
PTP-2O-S	4.0
PTP-4O-S	5.0
PTG-2O-S	5.0
PTG-4O-S	5.0
$\Sigma$	100.0

[0221] This mixture has the following properties:

Clearing point (T(N,I))° C.:	135.0
$n_e$ (20° C., 589.3 nm):	1.9906
$\Delta n$ (20° C., 589.3 nm):	0.4511

## Comparative Use-example 1

[0222] A liquid crystal mixture is realized consisting of:

Compound/Abbreviation	Concentration/mass-%
K6	12.0
K9	4.0
K15	29.6
M9	8.8
T15	8.0
PGIP-3-N	20.0
BB2I	5.6
BCH-5	12.0
$\Sigma$	100.0

[0223] This mixture has the following properties:

Clearing point (T(N,I))° C.:	113.0
$n_e$ (20° C., 589.3 nm):	1.8160
$\Delta n$ (20° C., 589.3 nm):	0.2860
$\epsilon_{  }$ (20° C., 1 kHz):	22.8
$\Delta\epsilon$ (20° C., 1 kHz):	17.3

## Comparative Use-example 2

[0224] A liquid crystal mixture is realized consisting of:

Compound/Abbreviation	Concentration/mass-%
ME2N.F	10.00
PPTUI-2-4	8.45
PPTUI-3-2	5.16
PPTUI-3-4	15.82
PPTUI-4-4	35.54
PPTUI-5-2	7.25
PPTUI-5-4	17.78
E	100.00

[0225] This mixture has the following properties:

Clearing point (T(N,I))/° C.:	145° C.
$\Delta n$ (20° C., 589.3 nm):	0.336
$\eta$ (20° C., 1 kHz):	9.8
$\Delta\epsilon$ (20° C., 1 kHz):	6.5

## Comparative Use-example 3

[0226] A liquid crystal mixture is realized consisting of:

Compound/Abbreviation	Concentration/mass-%
GGP-5-GL	16.0
PGIGI-3-CL	6.0
BCH-2.F.F	14.0
BCH-3.F.F	15.0
BCH-5.F.F	14.0
BCH-3.F.F.F	14.0
CGU-2-F	6.0
CGU-3-F	6.0
CGU-5-F	6.0
CBC-33F	3.0
E	100.0

[0227] This mixture has the following properties:

Clearing point (T(N,I))/° C.:	81.0
Smectic to nematic transition point (T(S, N))/° C.:	<-30
$n_e$ (20° C., 589.3 nm):	1.6711
$\Delta n$ (20° C., 589.3 nm):	0.1603
$\eta$ (20° C., 1 kHz):	14.6
$\Delta\epsilon$ (20° C., 1 kHz):	9.9

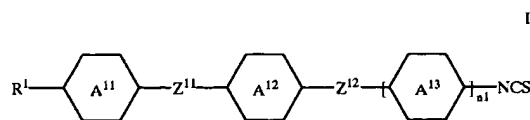
What is claimed is:

1. A liquid crystal medium, comprising:

a strongly dielectrically positive liquid crystal component A, containing one or more liquid crystal compounds with a terminal isothiocyanate group and having a  $\Delta n$  of more than 0.30 at 20° C. and 589.3 nm, and

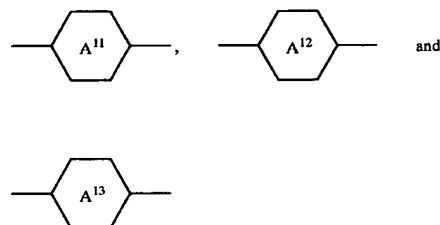
a dielectrically positive component B containing of one or more terminally polar substituted bi- or terphenyl compounds.

2. A liquid crystal medium according to claim 1, wherein the dielectrically positive liquid crystal component A comprises one or more compounds of formula I

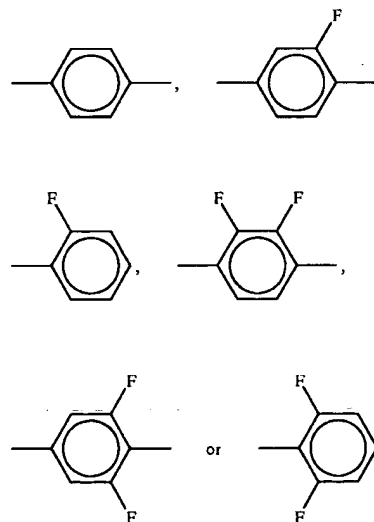


wherein

$R^1$  is n-alkyl, or n-alkoxy with 1 to 10 C-atoms, alkenyl, alkenyloxy or alkoxyalkyl with 2 to 7 C-atoms or CN, NCS, halogen, or alkyl, alkenyl, alkoxy, alkenyloxy or alkoxyalkyl substituted by one or more halogens,



Each, independently of each other, are



$Z^{11}$  and  $Z^{12}$  each are independent of each other a single bond or trans  $-\text{CH}=\text{CH}-$ , provided that when  $n^1$  is 0,  $Z^{12}$  is a single bond

$n^1$  is 0 or 1.